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Numerical Identification of Diffusivity Coefficient and Initial Condition by Discrete Mollification

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Abstract—We discuss the simultaneous identification of the initial condition and the space-time depending diffusivity coefficient for general linear one-dimensional parabolic equations when the measured information is obtained only at the active boundary.

We solve these problems by introducing stable space marching implementations of the Mollification Method which restore continuity with respect to the data. Several numerical examples show the properties of the methods.

Keywords—Ill-posed problem, Parabolic equations, Coefficient identification, Finite differences, Mollification method.

1. INTRODUCTION

The identification of diffusivity coefficients in parabolic equations is receiving considerable attention from researchers in a variety of fields. The use of space marching schemes, along with some kind of regularization, has proven to be an effective way of solving these ill-posed inverse problems. A finite differences space marching scheme with Hyperbolic Regularization, requiring the exact knowledge of the initial temperature distribution, was utilized by Ewing and Lin in [1] to identify a diffusivity coefficient that depends only on the space variable. The same identification problem, allowing for noisy initial and boundary data, was later investigated by Mejía and Murio in [2], with the introduction of a combined Mollification-Hyperbolic Regularization space marching algorithm.

In this paper, we present two stable space marching implementations of the Mollification Method that, based only on the availability of measured noisy boundary data, are able to numerically recover the space-time depending coefficients and, simultaneously, the missing initial condition associated with the direct problem.

Even though both space marching algorithms share the same underlying global philosophy, their numerical implementations are quite different depending on the formulation of the parabolic

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Typeset by $\mathcal{A}_{\mathcal{M}}\mathcal{S}$-TEX problem. We use one algorithm or the other, according to the diffusion process being described in divergence form or not.

The paper is organized as follows. Section 2 is a succinct review of basic results on the Mollification Method. Section 3 concentrates on the description of the coefficient identification problems and the numerical methods for their solutions. In Section 4, we consider the main properties of the numerical methods, and in Section 5, we present some illustrative numerical experiments.

2. MOLLIFICATION

Let

$$\rho_\delta(t) = \frac{1}{\delta\pi^{1/2}} \exp\left(\frac{-t^2}{\delta^2}\right).$$

The δ-mollification of a square integrable function $f(t)$ is given by the convolution

$$J_\delta f(t) = (\rho_\delta * f)(t) = \int_{-\infty}^{\infty} \rho_\delta(t-s) f(s)\, ds.$$

It satisfies the following estimates.

PROPOSITION 1.

a. *If $f(t) \in C^2(I)$, $I \subset R$, then there exists a constant C independent of δ such that*

$$\|J_\delta f - f\|_{\infty,I} \le C\delta \quad \text{and} \quad \|J_\delta f' - f'\|_{\infty,I} \le C\delta.$$

b. *If $f_m(t) \in C^0(I)$ and $\|f - f_m\|_{\infty,I} \le \epsilon$, then*

$$\|J_\delta f - J_\delta f_m\|_{\infty,I} \le \epsilon$$

and

$$\left\|(J_\delta f)' - (J_\delta f_m)'\right\|_{\infty,I} \le \left(\frac{2}{\sqrt{\pi}}\right)\frac{\epsilon}{\delta}.$$

PROOF. See [3].

3. THE IDENTIFICATION PROBLEMS

3.1. Preliminaries

Let $I = (0,1)$ and $D = I \times I$. We consider the following problems.

PROBLEM 1. *Identify $a(x,t)$, $(x,t) \in D$, and $u(x,0)$, $x \in I$, in*

$$\begin{aligned} u_t &= (au_x)_x + f(x,t), && (x,t) \in D,\\ u(0,t) &= \psi_m(t), && 0 < t,\\ u_x(0,t) &= \phi_m(t), && 0 < t,\\ a(x_0,t) &= \sigma_m^0(t), && 0 < t,\\ a(x_1,t) &= \sigma_m^1(t), && 0 < t, \end{aligned} \tag{1}$$

where $0 < x_0 < x_1 \ll 1$ and $\psi_m(t)$, $\phi_m(t)$, $\sigma_m^0(t)$, and $\sigma_m^1(t)$ are the measured noisy approximations of the exact data functions $\psi(t)$, $\phi(t)$, $\sigma^0(t)$, and $\sigma^1(t)$, satisfying $\|\psi - \psi_m\|_{\infty,I} \le \epsilon$, $\|\phi - \phi_m\|_{\infty,I} \le \epsilon$, and $\|\sigma^i - \sigma_m^i\|_{\infty,I} \le \epsilon$, $i = 0,1$, where ϵ is a positive tolerance. The coefficient histories at x_0 and x_1 play the role of the boundary values for the coefficient a. The selection of x_0 and x_1 is usually linked to the step size of the discretization in x in a way to be described later.

PROBLEM 2. *The second identification problem, previously considered in [4], is the following. Identify* $a(x,t)$, $(x,t) \in D$, *and* $u(x,0)$, $x \in I$, *in*

$$\begin{aligned} u_t &= a u_{xx} + f(x,t), && (x,t) \in D, \\ u(0,t) &= \psi_m(t), && 0 < t, \\ u_x(0,t) &= \phi_m(t), && 0 < t, \\ a(0,t) &= \sigma_m(t), && 0 < t, \end{aligned} \tag{2}$$

where $\psi_m(t)$, $\phi_m(t)$, *and* $\sigma_m(t)$ *are the measured approximations of the exact data functions* $\psi(t)$, $\phi(t)$, *and* $\sigma(t)$. *It is assumed that* $\|\psi - \psi_m\|_{\infty,I} \le \epsilon$, $\|\phi - \phi_m\|_{\infty,I} \le \epsilon$, *and* $\|\sigma - \sigma_m\|_{\infty,I} \le \epsilon$, *where* ϵ *is a positive tolerance.*

A variety of unknown coefficient problems for parabolic equations is presented in [3,5] and the references therein. Generally, inverse problems are ill-posed and coefficient identification problems are no exception. In order to restore continuity with respect to the data for problems (1) and (2), we develop space marching implementations of the Mollification Method. The regularization of (1) by the Mollification Method leads us to the following mollified problem.

PROBLEM 1$'$. *Identify* $a(x,t)$, $(x,t) \in D$, *and* $u(x,0)$, $x \in I$, *in*

$$\begin{aligned} u_t &= (a u_x)_x + f(x,t), && (x,t) \in D, \\ u(0,t) &= J_\delta \psi_m(t), && 0 < t, \\ u_x(0,t) &= J_\delta \phi_m(t), && 0 < t, \\ a(x_0,t) &= J_\delta \sigma_m^0(t), && 0 < t, \\ a(x_1,t) &= J_\delta \sigma_m^1(t), && 0 < t, \end{aligned} \tag{3}$$

where δ *is the radius of mollification, and* $J_\delta \psi_m(t)$, $J_\delta \phi_m(t)$, *and* $J_\delta \sigma_m^i(t)$, $i = 0, 1$, *are the mollifications in* t *of* $\psi_m(t)$, $\phi_m(t)$, *and* $\sigma_m^i(t)$, *respectively.*

The implementation of the Mollification Method for Problem (2) with measured data, leads us to the consideration of the following problem.

PROBLEM 2$'$. *Identify* $a(x,t)$, $(x,t) \in D$, *and* $u(x,0)$, $x \in (0,1)$, *in*

$$\begin{aligned} u_t &= a u_{xx} + f(x,t), && (x,t) \in D, \\ u(0,t) &= J_\delta \psi_m(t), && 0 < t, \\ u_x(0,t) &= J_\delta \phi_m(t), && 0 < t, \\ a(0,t) &= J_\delta \sigma_m(t), && 0 < t, \end{aligned} \tag{4}$$

where δ *is the radius of mollification, and* $J_\delta \psi_m(t)$, $J_\delta \phi_m(t)$, *and* $J_\delta \sigma_m(t)$ *are the mollifications in* t *of* $\psi_m(t)$, $\phi_m(t)$, *and* $\sigma_m(t)$, *respectively.*

For the solution u, the coefficient a and the forcing term f of the PDE (1), we make the following assumptions.

ASSUMPTION 1. *Let* $B = [0,1] \times [0,T]$, *where* T *depends on* h *and* k *in a way to be specified later.*

a. *(Regularity)* $u(x,t) \in C^2(B)$ *and* $a, f \in C^0(B)$.
b. *(Identifiability) There are constants* α_1 *and* β_1 *such that* $0 < \alpha_1 \le a(x,t)$ *and* $0 < \beta_1 \le |u_x(x,t)|$, $(x,t) \in B$.

The corresponding assumptions for Problem 2 are the following.

ASSUMPTION 2. *Let* $B = [0,1] \times [0,T]$, *where* T *depends on* h *and* k *in a way to be specified later.*

a. *(Regularity)* $u(x,t) \in C^2(B)$ *and* $a, f \in C^0(B)$.
b. *(Identifiability) There are constants* α_2 *and* β_2 *such that* $0 < \alpha_2 \le a(x,t)$ *and* $0 < \beta_2 \le |u_{xx}(x,t)|$, $(x,t) \in B$.

3.2. The Marching Schemes

Let M and N be positive integers, $h = 1/M$, $k = 1/N$.

PROBLEM 1$'$. *Denote* $x_j = (j + 1/2)\,h$, $j = 0, 1, \ldots, M-1$, $t_n = nk$, $n = 0, 1, \ldots$. *For* $n \geq 0$, *let*

$$\begin{aligned} u_0^n &= \psi(nk), & & \\ a_{1/2}^n &= \sigma^0(nk), & & \\ a_{3/2}^n &= \sigma^1(nk), & & \\ f_j^n &= f(jh, nk), & \qquad & j \geq 0, \\ u_j^n &= u(jh, nk), & & j \geq 1, \\ a_{j+1/2}^n &= a\left(\left(j + \frac{1}{2}\right) h, nk\right), & & j \geq 2. \end{aligned} \tag{5}$$

Let the discrete functions that define the numerical method be U_j^n *and* $A_{j+1/2}^n$. *Their starting values are given for all* n *in order to proceed with a space marching scheme. They are*

$$\begin{aligned} U_0^n &= J_\delta \psi_m(nk), \\ A_{1/2}^n &= J_\delta \sigma_m^0(nk), \\ A_{3/2}^n &= J_\delta \sigma_m^1(nk). \end{aligned} \tag{6}$$

The assumptions on u and a for Problem 1 have their corresponding ones for the discrete variables. They are the following.

ASSUMPTION 1$'$. *For all* j *and* n, *the discrete functions that define the numerical method for the solution of Problem 1$'$ satisfy:*

a. $0 < \alpha_1 \leq A_{j-1/2}^n$. *Moreover,* $2A_{j-1/2}^n - A_{j-3/2}^n$ *does not change sign and* $0 < \alpha_1 \leq |2A_{j-1/2}^n - A_{j-3/2}^n|$.
b. $U_{j+1}^n - U_{j-1}^n$ *does not change sign and* $0 < \beta_1 \leq |U_{j+1}^n - U_{j-1}^n|$.

The identification of the coefficient a is made through the Predictor-Corrector Scheme described in the following algorithm.

1. Compute U_1^n by the formula

$$U_1^n = U_0^n + hJ_\delta \phi_m(nk). \tag{7}$$

2. Compute U_2^n as in [1]; that is,

$$U_2^n = U_1^n + \frac{1}{A_{3/2}^n}\left[A_{1/2}^n\left(U_1^n - U_0^n\right) + h^2\left(\frac{U_1^{n+1} - U_1^{n-1}}{2k} - f_1^n\right)\right]. \tag{8}$$

3. For $j = 2, 3, \ldots, M-1$,
   - Predictor Step: Let

$$A_{j+1/2}^n = 2A_{j-1/2}^n - A_{j-3/2}^n. \tag{9}$$

   - Compute U_{j+1}^n by

$$U_{j+1}^n = U_j^n + \frac{1}{A_{j+1/2}^n}\left[A_{j-1/2}^n\left(U_j^n - U_{j-1}^n\right) + h^2\left(\frac{U_j^{n+1} - U_j^{n-1}}{2k} - f_j^n\right)\right]. \tag{10}$$

   - Compute U_{j+1}^0 by linear extrapolation.
   - Corrector Step: Compute $A_{j+1/2}^n$ by

$$\begin{aligned} A_{j+1/2}^n = \frac{1}{U_{j+1}^n - U_{j-1}^n}\Big[&A_{j-1/2}^n\left(-U_{j+1}^n + 4U_j^n - 3U_{j-1}^n\right) \\ &+ \frac{h^2}{k}\left(U_j^{n+1} - U_j^{n-1}\right) - 2h^2 f_j^n\Big]. \end{aligned} \tag{11}$$

   - Mollify $A_{j+1/2}^n$ as a discrete function of n.

REMARK. If we assume enough regularity on u and a, the differential equation in (1) can be written

$$u_t = a_x u_x + a u_{xx} + f. \tag{12}$$

By using the standard approximations

$$\begin{aligned} a(jh, nk) &= \frac{1}{2}\left(a_{j+1/2}^n + a_{j-1/2}^n\right) + O(h), \\ a_x(jh, nk) &= \frac{1}{h}\left(a_{j+1/2}^n - a_{j-1/2}^n\right) + O(h^2), \\ u_x(jh, nk) &= \frac{1}{h}\left(u_j^n - u_{j-1}^n\right) + O(h), \\ u_t(jh, nk) &= \frac{1}{2k}\left(u_j^{n+1} - u_j^{n-1}\right) + O(k^2) \end{aligned}$$

and

$$u_{xx}(jh, nk) = \frac{1}{h^2}\left(u_{j+1}^n - 2u_j^n + u_{j-1}^n\right) + O(h^2),$$

we easily find that

$$\begin{aligned} a_{j+1/2}^n = \frac{1}{u_{j+1}^n - u_{j-1}^n} &\Big[a_{j-1/2}^n\left(-u_{j+1}^n + 4u_j^n - 3u_{j-1}^n\right) \\ &+ \frac{h^2}{k}\left(u_j^{n+1} - u_j^{n-1}\right) - 2h^2 f_j^n\Big] + O(h) + O(k^2). \end{aligned} \tag{13}$$

This equation may be considered as a motivation for equation (11) of the numerical scheme presented above.

PROBLEM 2′. *Denote* $x_j = jh$, $j = 0, 1, \ldots, M$, $t_n = nk$, $n = 0, 1, \ldots$. *Let* $v(x,t) = u_x(x,t)$ *and* $w(x,t) = u_t(x,t)$. *For* $n \geq 0$, *let*

$$\begin{aligned} u_0^n &= \psi(nk), \\ a_0^n &= \sigma(nk), \\ v_0^n &= \phi(nk), \\ w_0^n &= \psi'(nk), \\ f_j^n &= f(jh, nk), \qquad j \geq 0, \\ u_j^n &= u(jh, nk), \qquad j \geq 1, \\ v_j^n &= v(jh, nk), \qquad j \geq 1, \\ w_j^n &= w(jh, nk), \qquad j \geq 1, \\ a_j^n &= a(jh, nk), \qquad j \geq 1. \end{aligned} \tag{14}$$

Let the variables of the numerical method be U_j^n, V_j^n, W_j^n, and A_j^n. They are discrete functions defined on the grid with discretization steps h and k. As for Problem 1′, their starting values are given for all n in order to proceed with a space marching scheme. They are

$$\begin{aligned} U_0^n &= J_\delta \psi_m(nk), \\ V_0^n &= J_\delta \phi_m(nk), \\ W_0^n &= (J_\delta \psi_m)'(nk), \\ A_0^n &= J_\delta \sigma_m(nk), \end{aligned}$$

and they satisfy the following hypotheses.

ASSUMPTION 2′. *For all j and n, the discrete functions that define the numerical method for the solution of Problem 2′ satisfy:*

a. $0 < \alpha_2 \leq A_j^n$.

b. $W_j^n - f_j^n$ *does not change sign and* $0 < \alpha_2\beta_2 \leq |W_j^n - f_j^n|$.

The space marching numerical scheme is defined by the equations

$$U_{j+1}^n = U_j^n + hV_j^n, \tag{15}$$

$$W_{j+1}^n = W_j^n + \frac{h}{k}\left(V_j^{n+1} - V_j^n\right), \tag{16}$$

$$V_{j+1}^n = V_j^n + \frac{h}{A_j^n}\left(W_j^n - f_j^n\right), \tag{17}$$

and

$$A_{j+1}^n = A_j^n \frac{\left(W_{j+1}^{n-1} - f_{j+1}^n\right)}{\left(W_j^n - f_j^n\right)}. \tag{18}$$

These equations are implemented according to the following algorithm. For $j = 0, 1, \dots, M-1$:

1. Compute U_{j+1}^n by (15) for $n = 1, 2, \dots, L+1-j$.
2. Compute U_{j+1}^0 by linear extrapolation.
3. Compute V_{j+1}^n by (17) for $n = 1, 2, \dots, L-j$.
4. Compute W_{j+1}^n by (16) for $n = 1, 2, \dots, L-j$.
5. Compute A_{j+1}^n by (18) for $n = 2, 3, \dots, L-j$.
6. Mollify A_{j+1}^n for $n = 2, 3, \dots, L-j$.
7. Compute A_{j+1}^1.

REMARK. The computations are performed in a triangular region in the (x,t)-plane and a sufficient amount $L+1$ of point values of the boundary data at $x = 0$ should be read. We link T and L by setting $(L+1)k = T$.

Some equations satisfied by the exact functions at the grid points (recall (14)) are essential now. They are at the same time, a motivation for the definition of the numerical scheme and an important step toward the proof of error estimates. The first one, similar to (15), is a first order Taylor expansion of the temperature solution $u(x,t)$; i.e.,

$$u_{j+1}^n = u_j^n + hv_j^n + O\left(h^2\right). \tag{19}$$

The second one, corresponding to (16), is a first order discretization of the equation $u_{tx} = u_{xt}$,

$$w_{j+1}^n = w_j^n + \frac{h}{k}\left(v_j^{n+1} - v_j^n\right) + O\left(h^2\right) + O(k), \tag{20}$$

and the third one, corresponding to (17), is an approximation of the differential equation in problem (2):

$$v_{j+1}^n = v_j^n + \frac{h}{a_j^n}\left(w_j^n - f_j^n\right) + O\left(h^2\right). \tag{21}$$

A motivation for equation (18) requires several steps:

1. First order discretization of the time derivative:

$$w_j^n = \frac{1}{k}\left(u_j^{n+1} - u_j^n\right) + O(k). \tag{22}$$

2. Centered difference approximation in space and time of the differential equation (2):

$$\frac{1}{2k}\left(u_j^{n+1} - u_j^{n-1}\right) - f_j^n = a_j^n\left(\frac{1}{2h}\left(v_{j+1}^n - v_{j-1}^n\right)\right) + O\left(h^2\right) + O\left(k^2\right). \tag{23}$$

3. Forward difference approximation in space and time of the differential equation (2):

$$\frac{1}{k}\left(u_j^{n+1} - u_j^n\right) - f_j^n = a_j^n\left(\frac{1}{h}\left(v_{j+1}^n - v_j^n\right)\right) + O(h) + O(k). \tag{24}$$

From equations (23) and (24), we obtain

$$\frac{1}{k}\left(u_{j+1}^n - u_{j+1}^{n-1}\right) - f_{j+1}^n = a_{j+1}^n\left(\frac{1}{h}\left(v_{j+1}^n - v_j^n\right)\right) + O(h) + O(k),$$

and combining this equation with (22) and (24), we get

$$a_{j+1}^n = a_j^n \frac{\left(w_{j+1}^{n-1} - f_{j+1}^n\right)}{\left(w_j^n - f_j^n\right)} + O(h) + O(k). \tag{25}$$

4. PROPERTIES OF THE NEW METHODS

This section discusses the numerical stability of the algorithms described in the previous section as well as an error analysis that shows the restoration of continuity with respect to the data. We begin with the definition of maximum norms for discrete functions. Let G_j^n be a discrete function. We define

$$|G_j| = \max_n |G_j^n|$$

and

$$\|G\|_\infty = \max_j |G_j| .$$

4.1. Stability

The stability of the numerical method for the solution of Problem 1′ is described by the following theorem.

THEOREM 1. *If Assumptions 1 and 1′ hold and there exists a constant d such that $k = dh$, then $\|A\|_\infty$ and $\|U\|_\infty$ are finite.*

PROOF. The proof is by induction.

We notice first that U_0^n, U_1^n, $A_{1/2}^n$, and $A_{3/2}^n$ are bounded discrete functions of n. Suppose U_{i+1}^n and $A_{i+1/2}^n$ are bounded discrete functions of n for $i = 1, 2, \dots, j-1$. Let us prove that $|U_{j+1}|$ and $|A_{j+1/2}|$ are finite.

By looking at (10), we observe that, for all n,

$$\left|U_{j+1}^n\right| \le |U_j| + \frac{1}{\alpha}\left[\left|A_{j-1/2}\right|\left(|U_j| + |U_{j-1}|\right) + \frac{h^2}{k}|U_j| + h^2\|f\|_\infty\right]. \tag{26}$$

By induction hypothesis, $|U_{j+1}|$ is finite.

Analogously, equation (11) and Assumption 1′ imply that, for all n,

$$\left|A_{j+1/2}^n\right| \le \frac{1}{\beta}\left[\left|A_{j-1/2}\right|\left(|U_{j+1}| + 4|U_j| + 3|U_{j-1}|\right) + \frac{2h}{d}|U_j| + 2h^2\|f\|_\infty\right], \tag{27}$$

which, by using (26) and the induction hypothesis, allows us to conclude that $|A_{j+1/2}|$ is finite. ∎

REMARK. The mollified coefficient will satisfy the same estimate with the addition of an $O(\delta)$ term.

The analogous stability estimate for Problem 2′ is presented in the following theorem.

THEOREM 2. *If Assumptions 2 and 2′ hold, and there are constants d_1 and d_2 such that $\max\{h, (h/\alpha)\} \le d_1$ and $2h/k \le d_2$, then $\|V\|_\infty$, $\|U\|_\infty$, $\|W\|_\infty$, and $\|A\|_\infty$ are finite.*

PROOF. See [4].

4.2. Error Analysis

PROBLEM 1′. *We begin by defining the following discrete error functions:*

$$\begin{aligned}
\Delta U_j^n &= u_j^n - U_j^n, \\
\Delta A_{j+1/2}^n &= a_{j+1/2}^n - A_{j+1/2}^n, \\
E_j &= \left|\Delta U_j^n\right| + \left|\Delta A_{j-1/2}^n\right| .
\end{aligned}$$

It is easily shown that the error in the mollified diffusion coefficient is of the form $|\Delta A_{j-1/2}^n| + C\delta$. Therefore, we focus our attention on the first term of this error.

The discrete error functions E_1 and E_2 represent the initial error for our numerical scheme. They satisfy the following estimate.

LEMMA 1. *If the hypotheses of Theorem 1 hold, then there exist constants C_1, C_2, and C_3 such that*

$$E_1 + E_2 \leq C_1\delta + C_2\epsilon + C_3 h.$$

PROOF. Apply Proposition 1 to the errors ΔU_1^n, ΔU_2^n, $\Delta A_{1/2}^n$, and $\Delta A_{3/2}^n$. The first two errors are readily obtained from (5), (7), and (8). The last two errors come directly from (5) and (6). ∎

The next theorem shows the restoration of continuity with respect to the data.

THEOREM 3. *If Assumptions 1 and 1′ hold and there exists a constant d such that $k = dh$, then there exists a constant C such that*

$$E_j + E_{j+1} \leq C\left(E_{j-1} + E_j\right) + O(h), \qquad j = 2, 3, \dots, M-1.$$

PROOF. Standard discrete approximations of the PDE (1) and equation (10) imply that

$$\begin{aligned}\left(2A_{j-1/2}^n - A_{j-3/2}^n\right)\Delta U_{j+1}^n = {} & \left(u_{j+1}^n - u_j^n\right)\Delta A_{j-3/2}^n + \left(-2u_{j+1}^n + 3u_j^n - u_{j-1}^n\right)\Delta A_{j-1/2}^n \\ & + \left(3A_{j-1/2}^n - A_{j-3/2}^n\right)\Delta U_j^n - A_{j-1/2}^n \Delta U_{j-1}^n \\ & + \frac{h^2}{k}\left(\Delta U_j^{n+1} - U_j^{n-1}\right) + O(h),\end{aligned}$$

which, by using Assumption 1′ and Theorem 1, yields the estimate

$$\begin{aligned}\left|\Delta U_{j+1}\right| \leq \frac{1}{\alpha}\Bigg[& 2\left\|u\right\|_\infty \left|\Delta A_{j-3/2}\right| + 6\left\|u\right\|_\infty \left|\Delta A_{j-1/2}\right| + 4\left\|A\right\|_\infty \left|\Delta U_j\right| \\ & + \left\|A\right\|_\infty \left|\Delta U_{j-1}\right| + \frac{h}{d}\left|\Delta U_j\right|\Bigg] + O(h).\end{aligned}$$

So, there is a constant C_1 such that

$$\left|\Delta U_{j+1}\right| \leq C_1\left(E_j + E_{j-1}\right) + O(h). \tag{28}$$

The estimate for the diffusion coefficient is obtained in analogous way. The conclusion is that there exists a constant C_2 so that

$$\left|\Delta A_{j+1/2}\right| \leq C_2\left(E_j + E_{j-1}\right) + O(h). \tag{29}$$

The result follows from (28) and (29). ∎

COROLLARY 1. *Under the hypotheses of Theorem 3, there exists a constant C such that*

$$\left\|E\right\|_\infty \leq C\left(E_1 + E_2\right).$$

PROOF. Let $T_j = E_j + E_{j-1}$. By Theorem 3, there exists a constant C so that

$$E_j \leq T_j \leq CT_{j-1} + O(h).$$

We assume $T_j > 0$ for all j. Thus, there exists B_{j-1} such that

$$T_j \leq B_{j-1}T_{j-1}(1 + O(h)).$$

If $B = \max_{1 \le i \le M} B_i$, we have $T_j \le B^M T_2 \exp(C_0)$, for some constant C_0, and the desired result follows with $C = B^M \exp(C_0)$. ∎

PROBLEM 2'. *In this case, the error analysis is based on the following discrete error functions:*

$$\begin{aligned}
\Delta U_j^n &= u_j^n - U_j^n, \\
\Delta A_j^n &= a_j^n - A_j^n, \\
\Delta V_j^n &= v_j^n - V_j^n, \\
\Delta W_j^n &= w_j^n - W_j^n, \\
E_j &= |\Delta U_j| + |\Delta A_j| + |\Delta V_j| + |\Delta W_j|.
\end{aligned}$$

The measured approximations at the active boundary are responsible for the error E_0. By using Proposition 1, it is readily seen that there is a constant C such that

$$E_0 \le C\left(\epsilon + \delta + \frac{\epsilon}{\delta}\right). \tag{30}$$

The restoration of continuity with respect to the data is summarized in the following theorem.

THEOREM 4. *If Assumptions 2 and 2' hold, and there are constants d_2, d_3, and d_4 such that $2h/k \le d_2$, $k = d_4 h$, and $\max\{h, (h/\alpha^2)\} \le d_3$, then there exists a constant C such that*

$$\|E\|_\infty \le C E_0.$$

PROOF. See the Appendix.

5. NUMERICAL RESULTS

In this section, we discuss the implementation of the new algorithms and present the numerical results from several examples.

The discrete error functions are measured by means of the weighted l^2-norms defined as follows:

- If G_j is a discrete function of j, $j = 1, 2, \ldots, M$, then its weighted l^2-norm is given by

$$\|G\|_2 = \left[\frac{1}{M}\sum_{j=1}^{M} |G_j|^2\right]^{1/2}.$$

- If G_j^n is a discrete function of j and n, $j = 1, 2, \ldots, M$, and $n = 1, 2, \ldots, N$, its weighted l^2-norm is given by

$$\|G\|_2 = \left[\frac{1}{MN}\sum_{j=1}^{M}\sum_{n=1}^{N} |G_j^n|^2\right]^{1/2}.$$

In all cases, the discretized measured approximations of the boundary data are simulated by adding random errors to the exact data at every grid point (j, n); i.e., if G_j^n denotes the exact discrete function, the measured grid function $G_{m,j}^n$ is given by

$$G_{m,j}^n = G_j^n + \varepsilon_j^n,$$

where the ε_j^n are independent Gaussian variables with constant variance $\sigma^2 = \epsilon^2$ and zero mean.

The stability and accuracy of the algorithms for the numerical solution of Problems 1 and 2 are tested for different average perturbations ϵ and appropriate values of the mollification radius δ.

Table 1. Error norms as functions of ϵ in Example 1a.

ϵ	δ	$\|\Delta A\|_2$	$\|\Delta U^0\|_2$
0.000	0.000	0.0363	0.0084
0.003	0.025	0.0456	0.0316
0.005	0.050	0.0715	0.0417

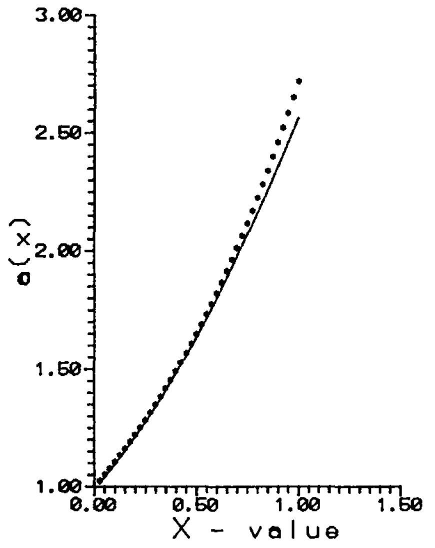

Figure 1. Initial condition in Example 1a. $\epsilon = 0.005$, $\delta = 0.05$. Exact: $(* * *)$; Computed: (—).

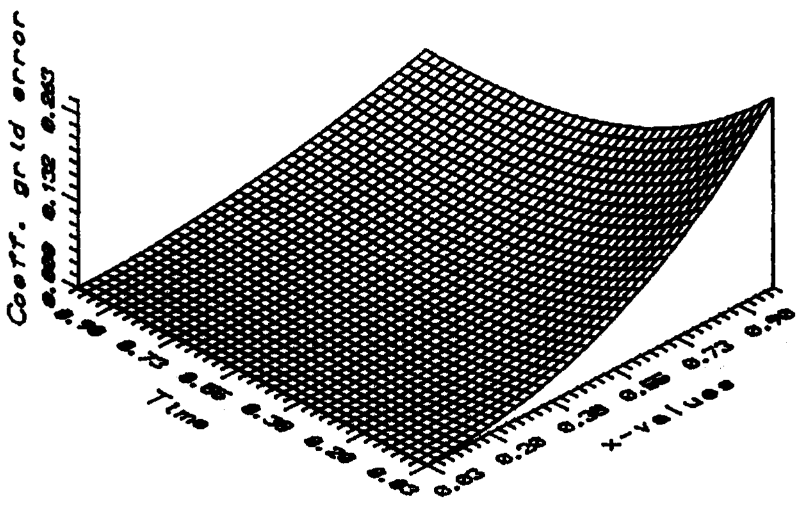

Figure 2. Error in $a(x,t)$. Example 1a. $\epsilon = 0.005$, $\delta = 0.05$.

Problem 1

EXAMPLE 1a. Identify $a(x,t)$ and $u(x,0)$ in

$$\begin{aligned} u_t &= (au_x)_x + f(x,t), && 0 < x < 1, \quad 0 < t, \\ u(0,t) &= \exp(-t), && 0 < t, \\ u_x(0,t) &= \exp(-t), && 0 < t, \\ a\left(\frac{1}{80}, t\right) &= 1 + \frac{1}{160}t, && 0 < t, \end{aligned}$$

Table 2. Error norms as functions of ϵ in Example 1a.

ϵ	δ	$\|\Delta A\|_2$	$\|\Delta U^0\|_2$
0.000	0.000	0.1170	0.0528
0.003	0.075	0.0924	0.0065
0.005	0.125	0.0935	0.0158

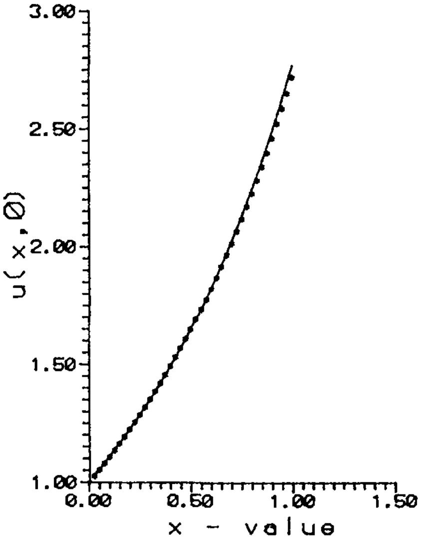

Figure 3. Initial condition in Example 1b. $\epsilon = 0.005$, $\delta = 0.125$. Exact: $(* * *)$; Computed: (—).

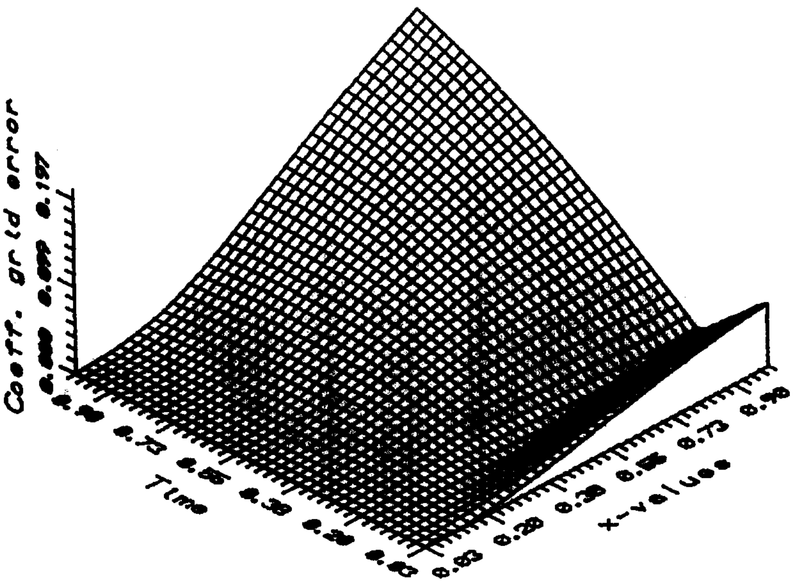

Figure 4. Error in $a(x,t)$. Example 1b. $\epsilon = 0.005$, $\delta = 0.125$.

$$a\left(\frac{3}{80}, t\right) = 1 + \frac{3}{160}t, \qquad 0 < t,$$

where $f(x,t) = -(2 + (t/2)(x+1))\exp(x-t)$.

The exact solutions are

$$a(x,t) = 1 + \frac{1}{2}xt \quad \text{and} \quad u(x,0) = \exp(x).$$

Table 3. Error norms as functions of ϵ in Example 2a.

Relative Errors			
ϵ	δ	$\|\Delta A\|_2$	$\|\Delta U^0\|_2$
0.000	0.020	0.0018	0.0054
0.003	0.100	0.0354	0.0042
0.005	0.140	0.0447	0.0037

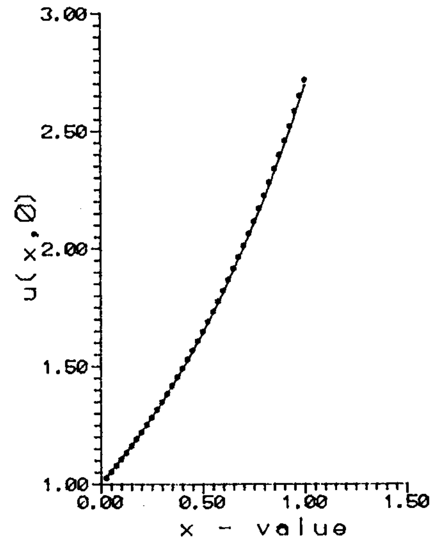

Figure 5. Initial condition in Example 2a. $\epsilon = 0.005$, $\delta = 0.05$. Exact: $(***)$; Computed: (—).

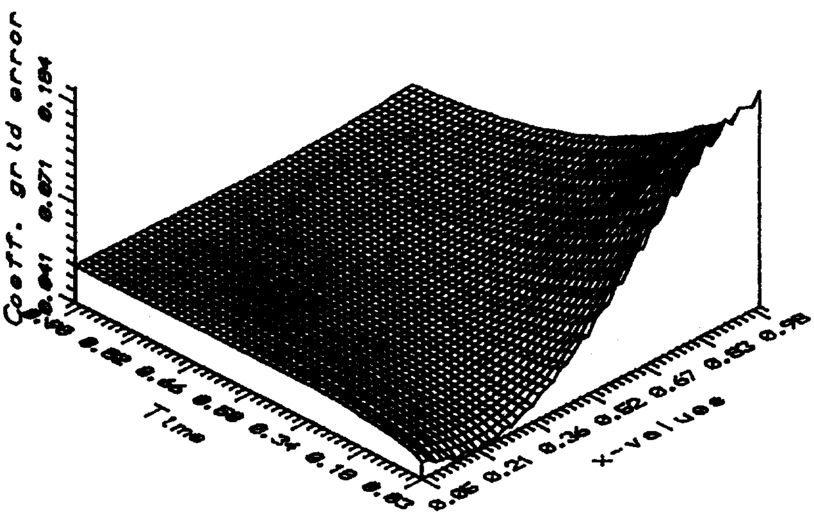

Figure 6. Error in $a(x,t)$. Example 2a. $\epsilon = 0.005$, $\delta = 0.05$.

Table 1 shows the discrete errors as functions of the amount of noise in the data ϵ for $M = N = 40$. The qualitative behavior of the reconstructed functions is shown in Figures 1 and 2.

EXAMPLE 1b. Identify $a(x,t)$ and $u(x,0)$ in

$$\begin{aligned} u_t &= (au_x)_x + f(x,t), && 0 < x < 1, \quad 0 < t, \\ u(0,t) &= \exp(t), && 0 < t, \\ u_x(0,t) &= \exp(t), && 0 < t, \end{aligned}$$

Table 4. Error norms as functions of ϵ in Example 2b.

Relative Errors			
ϵ	δ	$\|\Delta A\|_2$	$\|\Delta U^0\|_2$
0.000	0.010	0.0170	0.0031
0.003	0.050	0.1369	0.0262
0.005	0.050	0.1487	0.0283

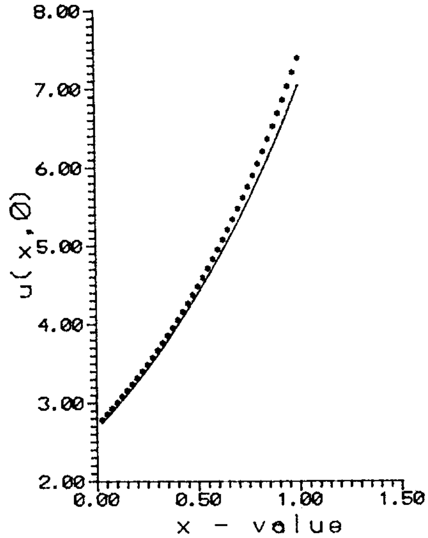

Figure 7. Initial condition in Example 2b. $\epsilon = 0.005$, $\delta = 0.125$. Exact: $(***)$; Computed: (—).

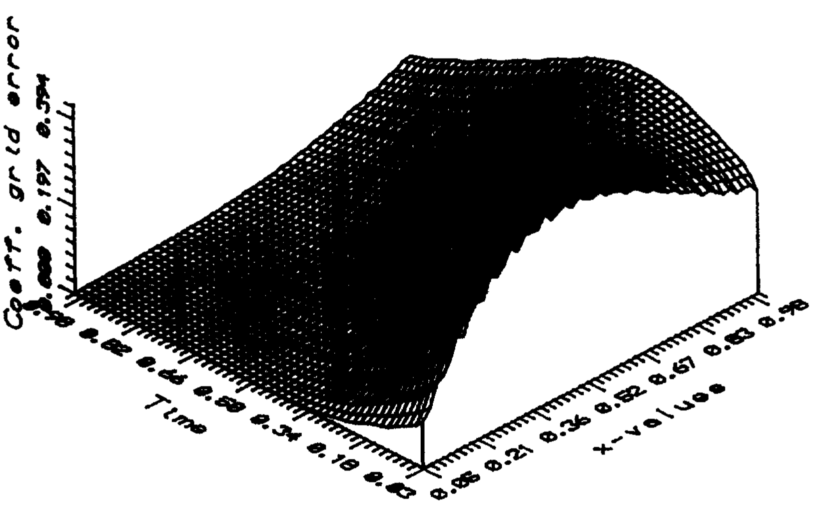

Figure 8. Error in $a(x,t)$. Example 2b. $\epsilon = 0.005$, $\delta = 0.125$.

$$a\left(\frac{1}{80}, t\right) = 1 + (\exp(-t))\left(\sin\frac{1}{80}\right), \qquad 0 < t,$$
$$a\left(\frac{3}{80}, t\right) = 1 + (\exp(-t))\left(\sin\frac{3}{80}\right), \qquad 0 < t,$$

where $f(x,t) = -(\exp(-t))(\sin x + \cos x)\exp(x+t)$.

The exact solutions are

$$a(x,t) = 1 + (\exp(-t))(\sin x) \quad \text{and} \quad u(x,0) = \exp(x).$$

We select $M = N = 40$. Table 2 and Figures 3 and 4 illustrate the quality of the reconstructions.

Problem 2

EXAMPLE 2a. Identify $a(x,t)$ and $u(x,0)$ in

$$\begin{aligned} u_t &= au_{xx} + f(x,t), && 0 < x < 1, \quad 0 < t, \\ a(0,t) &= 1 + 0.01t, && 0 < t, \\ u(0,t) &= \exp(t), && 0 < t, \\ u_x(0,t) &= \exp(t), && 0 < t, \end{aligned}$$

where $f(x,t) = -0.01(x+t)\exp(x+t)$.

The exact solutions are

$$a(x,t) = 1 + 0.01(x+t) \quad \text{and} \quad u(x,0) = \exp(x).$$

Table 3 shows the discrete relative errors as functions of the amount of noise in the data ϵ for $M = N = 50$. The qualitative behavior of the reconstructed functions is shown in Figures 5 and 6. The parameters for this experiment are $\epsilon = 0.005$ and $\delta = 0.12$.

EXAMPLE 2b. Identify $a(x,t)$ and $u(x,0)$ in

$$\begin{aligned} u_t &= au_{xx} + f(x,t), && 0 < x < 1, \quad 0 < t, \\ a(0,t) &= 1 && 0 < t, \\ u(0,t) &= \exp(1-t), && 0 < t, \\ u_x(0,t) &= \exp(1-t), && 0 < t, \end{aligned}$$

where $f(x,t) = -(2 + 0.1xt)\exp(1 + x - t)$.

The exact solutions are

$$a(x,t) = 1 + 0.1xt \quad \text{and} \quad u(x,0) = \exp(1+x).$$

We set $M = N = 100$. Table 4 illustrates the stability of the method by showing the relative errors as functions of the amount of noise in the data ϵ. The quality of the reconstructions can be observed in Figures 7 and 8, in which $\epsilon = 0.005$ and $\delta = 0.05$.

APPENDIX

With completeness in mind, we present a detailed proof of Theorem 4.

THEOREM. *If Assumptions 2 and 2′ hold, and there are constants d_2, d_3, and d_4 such that $2h/k \le d_2$, $k = d_4 h$ and $\max\{h, (h/\alpha^2)\} \le d_3$, then there exists a constant C_2 such that*

$$\|E\|_\infty \le C_2 E_0. \tag{31}$$

PROOF. Subtracting (17) from (21), we obtain

$$\Delta V_{j+1}^n = \Delta V_j^n + \frac{h}{a_j^n}\left(w_j^n - f_j^n\right) - \frac{h}{A_j^n}\left(W_j^n - f_j^n\right) + O(h^2).$$

Since

$$\frac{h}{a_j^n}\left(w_j^n - f_j^n\right) - \frac{h}{A_j^n}\left(W_j^n - f_j^n\right) = \frac{h}{a_j^n A_j^n}\left(A_j^n \Delta W_j^n - W_j^n \Delta A_j^n + f_j^n \Delta A_j^n\right),$$

then

$$\left|\Delta V_{j+1}^n\right| \le |\Delta V_j| + d_3 \left[\|A\|_\infty |\Delta W_j| + (\|W\|_\infty + \|f\|_\infty) |\Delta A_j|\right] + O\left(h^2\right),$$

and this implies

$$|\Delta V_{j+1}| \le C_3 E_j + O\left(h^2\right), \tag{32}$$

where $C_3 = \max\{1, d_3 \|A\|_\infty, d_3 (\|W\|_\infty + \|f\|_\infty)\}$.

Subtracting (16) from (20), we find

$$\Delta W_{j+1}^n = \Delta W_j^n + \frac{h}{k}\left(\Delta V_j^{n+1} - \Delta V_j^n\right) + O(h^2) + O(k).$$

This implies

$$\left|\Delta W_{j+1}^n\right| \le |\Delta W_j| + \frac{2h}{k} |\Delta V_j| + O\left(h^2\right) + O(k),$$

which provides an estimate of the form

$$|\Delta W_{j+1}| \le C_4 E_j + O\left(h^2\right) + O(k). \tag{33}$$

Now, from (18) and (25), we get

$$\Delta A_{j+1}^n \left(W_j^n - f_j^n\right) = -a_{j+1}^n \Delta W_j^n + \Delta A_j^n \left(W_{j+1}^{n-1} - f_{j+1}^n\right) + a_j^n \Delta W_{j+1}^{n-1} + O(h) + O(k).$$

By Assumption 2′,

$$\alpha\beta \left|\Delta A_{j+1}^n\right| \le \|a\|_\infty (2 |\Delta W_j| + d_2 |\Delta V_j|) + (\|W\|_\infty + \|f\|_\infty) |\Delta A_j| + O(h) + O(k),$$

which indicates that we can find a constant C_5 such that

$$|\Delta A_{j+1}| \le C_5 E_j + O(h) + O(k). \tag{34}$$

Finally, subtracting (15) from (19), we readily obtain the estimate

$$|\Delta U_{j+1}| \le C_6 E_j + O\left(h^2\right). \tag{35}$$

Now, we add inequalities (32)–(35) and make use of the hypothesis $k = d_4 h$ to get the estimate

$$E_{j+1} \le C_7 E_j + O(h),$$

where $C_7 = C_3 + C_4 + C_5 + C_6$. Without loss of generality, we assume $E_j > 0$. The ideas in the proof of Corollary 1 allow us to conclude the desired result. We state, for future reference, that the constant C_2 is of the form $C_2 = B^M \exp(C_0)$, for some constants B and C_0. ∎

A theoretical convergence result as the maximum noise in the data, ϵ, tends to 0, is easily obtained from the estimate (31).

COROLLARY. *If the hypotheses of Theorem 4 hold, then*

$$\lim_{\epsilon \to 0} \|E\|_\infty = 0.$$

PROOF. Recalling (30) and the fact that $C_2 = B^M \exp(C_8)$, we can write

$$\|E\|_\infty \le C_9 B^{1/h} \left(\epsilon + \delta + \frac{\epsilon}{\delta}\right)$$

for some constant C_9 independent of ϵ, δ, h, and k.

Let $\delta = \epsilon^{1/2}$ and $h = -(\ln B)/(\ln \epsilon^\eta)$, where $0 < \eta < 1/2$. Clearly, if ϵ tends to 0, so do δ and h. Since $B^{1/h} = \epsilon^{-\eta}$, then

$$\|E\|_\infty \le C_9 \epsilon^{-\eta} \left(\epsilon + 2\epsilon^{1/2}\right),$$

which tends to 0 as ϵ tends to 0. ∎

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